Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

Promising half-metallicity in ductile NbF_3: A first-principles prediction

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Table S1 The convergence of k-point mesh.

K-points	Energy(eV/atom)
5×5×5	-6.4769
7×7×7	-6.4710
9×9×9	-6.4733
11×11×11	-6.4754
13×13×13	-6.4762
15×15×15	-6.4757
17×17×17	-6.4760
3×3×5	-6.4783
3×3×7	-6.4735
5×5×9	-6.4748
5×5×11	-6.4764
7×7×13	-6.4755
7×7×15	-6.4757

Table S2 The convergence of energy cutoff of the plane waves.

ENCUT(eV)	Energy(eV/atom)
400	-6.4868
420	-6.4817
440	-6.4767
460	-6.4772
480	-6.4755
500	-6.4753
520	-6.4754

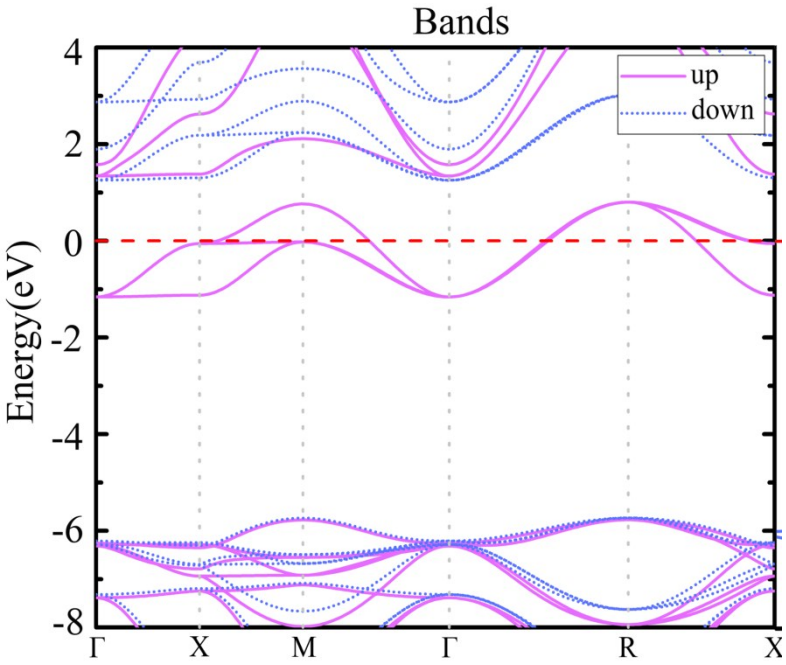

Fig. S1 The spin-resolved electronic band structure of NbF_3 obtained by using the GGA+U method. The energy at the Fermi level was set to zero.

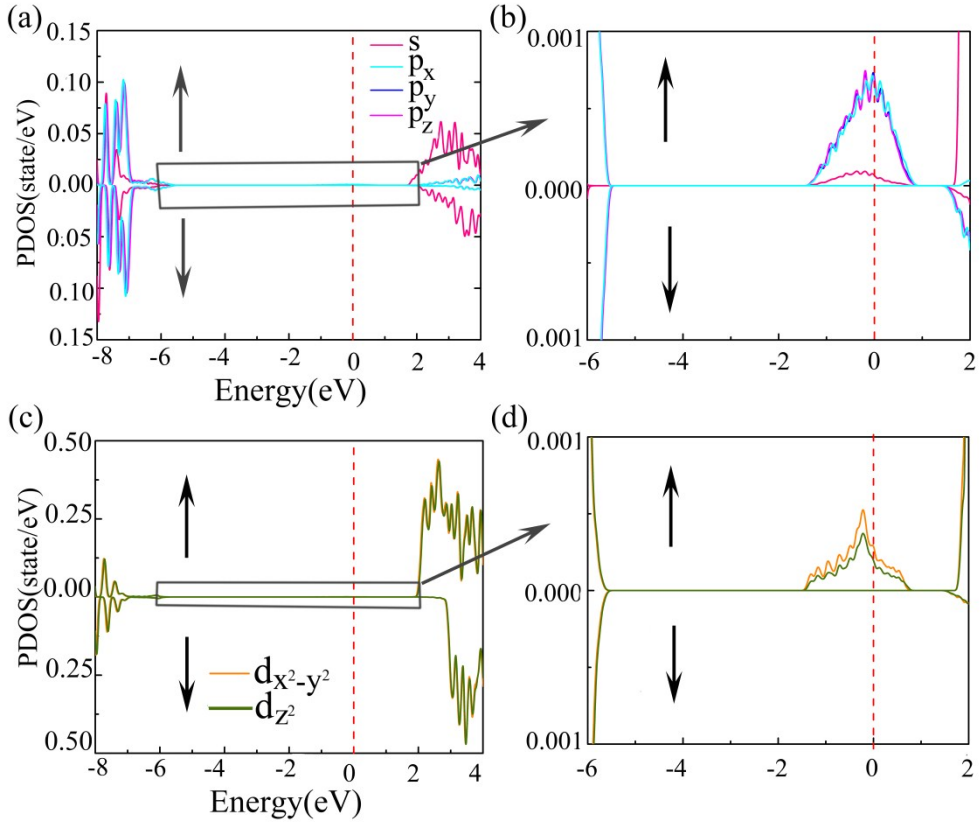

Fig. S2 (a) and (c) The s, p_x, p_y, p_z, d_{z2} and d_{x2-y2} orbital-resolved electron density of states (PDOS) projected onto Nb atom. (b) and (d) The enlarged view of the black box. The Fermi level was set to zero.The up and down arrows represent spin up and spin down, respectively.

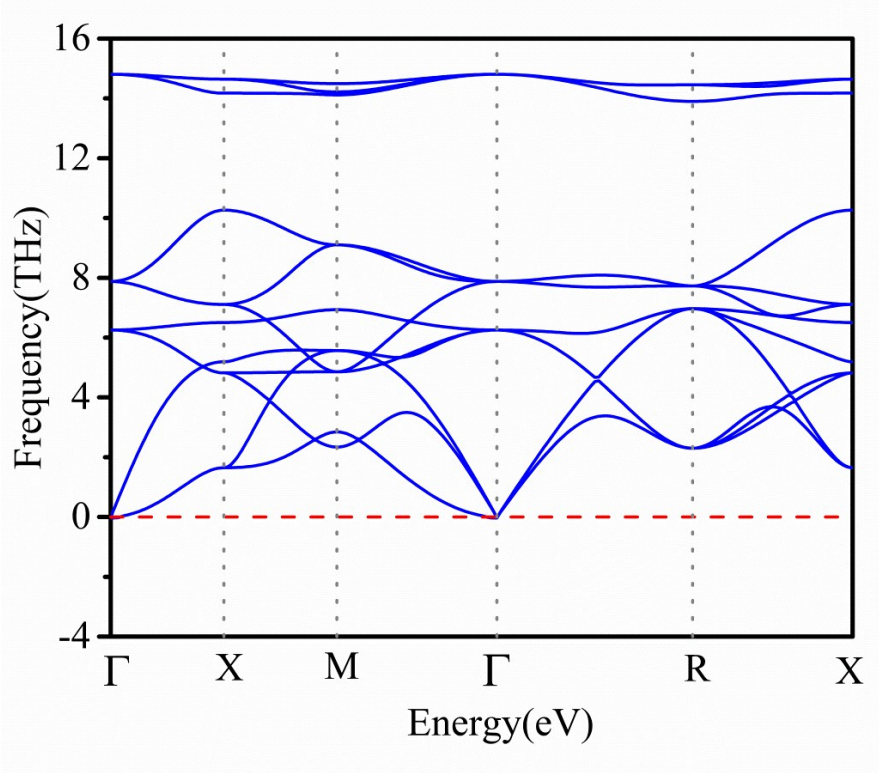

Fig. S3 The phonon spectrum of NbF_3 obtained by using a supercell approach within the PHONON code[1,2]. All the modes have positive frequencies in the BZ.

Reference

1. K. Parlinski, Z.Q. Li, Y. Kawazoe, *Phys. Rev. Lett., 1997,* **78**, 4063-4066.

2. D. Alfe,*Comput. Phys. Commun.,* 2009, **180** 2622-2633.